Mass Spectrometry PittCon® 2008

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The 59th Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (officially referred to as PittCon Conference & Expo 2008) was held March 1–7, 2008, at the newly remodeled Ernest N. Morial Convention Center in a much more subdued New Orleans, LA, than years past. The attendance at this year's conference was 19,536 (10,677 non-exhibitors and 8,859 exhibitors); this was a nearly 13% decrease from the 2007 attendance in Chicago of 22,426 and on a par with the Orlando 2006 attendance of 19,671. The last time PittCon was held in New Orleans, 2002, the attendance was 23,319. This year, there were 1,110 exhibitors (a 2.4% increase over last year) occupying 2,457 booths (a 3.4% increase). First-time exhibitors accounted for 15% of the total. The smaller attendance may have something to do with the increased difficulty to get to New Orleans. In previous years, there were at least one or two non-stop flights a day from San Francisco to New Orleans on United Airlines. Now there are only connection flights through Denver, Los Angles, and Chicago. There were far fewer people in the French Quarter restaurants than was the case in PittCons of the past. The city is still struggling to come back after the devastation of hurricane Katrina.

PittCon 2009 will be held March 8–13 at McCormick Place, Chicago, long before the start of spring on the Great Lakes. However, it will be easier to get to Chicago than it was to get to New Orleans unless the airport is closed because of weather. In researching this article, a copy of an *Analytical Chemistry* A-Pages article by Britt E. Erickson from March 2000 ("Pittcon Faces New Challenges: Exhibitors love it and hate it, and still find many reasons to go" *Anal. Chem.* **2000**, *72(5)*, 192A–196A) was discovered which accurately stated that PittCon would be in Chicago in 2004; but quoting Hyman Schultz, president of Pittcon 2000, "PittCon is going to Anaheim, CA, in 2009 to see what we are missing on the west coast." I wonder what happened.

Mass spectrometry did not have a year of new developments that have been seen at the last few PittCons. No mass spectrometry products received any of the *PittCon Editors' Awards*[1]. This may be due, in part, to my absence for the awards selections this year. I had to leave the conference early because I was one of those who came down with a strain of influenza that was not covered by this year's flu vaccine.

Companies like Thermo Fisher announced new models of existing products such as their GC/MS line, the shipping of electron transfer dissociation on the orbitrap (availability announced at ASMS in 2007 and which was the 2007 recipient of the Silver *PittCon Editors' Award* in 2007 for its implementation on the LTQ), and a new MALDI source for their orbitrap and LTQ-FT mass spectrometer. Waters introduced a version of the *Synapt™ HDMS™* (shown at Pittcon for the first time in 2007 and receiving the Gold *PittCon Editors' Award*) without the ion mobility feature, the *Synapt MS System*, which is field upgradable to the ion mobility version of the *Synapt HDMS*. Varian introduced a hybrid instrument using their triple quadrupole mass spectrometer and the FTICR instrument technology acquired from Ion Spec two years ago. Agilent introduced a new model of its triple quadrupole tandem-in-space MS/MS instrument (the *6410B*), GC × GC (2D GC) that does not require cryogenic cooling for use with their *7890A/5975C* gas chromatograph-mass spectrometer, a new version of the deconvolution report software (*DRS A.04.00*), and a new *Triple-Axis Detector* for the *5975C* that provides a signal-to-background of 400:1 for 1 pg of octafluoronaphthalene. As always, Bruker Daltonics introduced a number of new instruments and enhancements to existing mass spectrometers. Shimadzu and Shimadzu/Kratos exhibited enhancements to their GC/MS and LC/MS instruments as well as their MALDI TOF line. Applied Biosystems/MDS Sciex exhibited their *4000 QTRAP* (using properties of both a triple quadrupole and linear ion trap) with *LightSight 2.0* software. LECO Corp. (St. Joseph, MI) (http://www.LECO.com) showed for the first time at PittCon their new benchtop EI/CI unit resolution TOF GC-MS, the *TruTOF™ HT TOFMS*, which was introduced at ASMS in 2007 in addition to their line of GC × GC instruments, the *Pegasus® HT GC-MS* and the *Unique® HT TOFMS* liquid chromatograph-mass spectrometer. DANI Instruments S.p.A. (Viale Brianza, Italy), known for its gas chromatography products since 1975, showed a TOF-based GC-MS, the *Master TOFMS*. Advanced Chemistry Development (ACD/Labs) (http://www.acdlabs.com) introduced its ACD/*AutoChrom* for ChemStation (Agilent Technologies) and *Empower 2™* (Waters Corp.), a software-based automated method development system for HPLC, UHPLC, and LC/MS. Hitachi High Technologies America, Inc. (http://www.hitachi-hta.com/lcms) introduced its *NanoFrontier*, an integrated NanoLC and tandem-in-space linear quadrupole ion trap, in combination with a TOF *m/z* analyzer that is capable of Electron Capture Dissociation (ECD) – first non-FTICR instrument to have this feature.

[1] This award had its origin with *Analytical Instrument Industry Report*, Dr. Gordon Wilkinson, Founding Editor, in 1995. Since that time, many mass spectrometry products have received the Gold, Silver, and Bronze awards. 2004 was the first, and only, year that no award was received by a mass spectrometry product until now.

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It was also interesting to note that John Wiley & Sons continues to grow in mass spectrometry with the introduction of a number of book titles and a series of boutique electron ionization mass spectral databases.

Although not having new products as such, many of the companies from previous years returned with products. These companies included Cerno Bioscience (http://www.cernobioscience.com) with its software to provide accurate mass measurements from unit mass data; JEOL USA, Inc. (http://www.jeolusa.inc) with the DART (ion source) *AccuTOF* mass spectrometer; Prosolia, Inc. (http://www.prosolia.com) with their add-on desorption electrospray ionization (DESI) interface for various mass spectrometers; Ion Signature Technology, Inc. (http://www.ionsigtech.com) with their quantitation deconvolution software. Perkin Elmer Life and Analytical Sciences, Inc. (http://las.perkinelmer.com) continued the theme introduced last year at PittCon of emphasizing solutions rather than instruments with the introduction of the *EcoAnalytix* Melamine Analyzer, based on their *Clarus® 600T* GC-MS. IonSense, Inc. (http://www.ionsense.com) exhibited the DART ion source as an add-on for many mass spectrometers in the LEAP Technologies, Inc. booth (http://www.leaptec.com), their U.S. distributor; LEAP also exhibited its specialty sample introduction systems of GC/MS, LC/MS, and other instrumental purposes. LEAP also provides automation for the DART ion source. Torion Technologies (http://www.torion.net) with the *GUARDION™* portable GC-TMS, a toroidal quadrupole ion trap, and Lab Cyte (http://www.labcyte.com) with their innovative *630 MALDI Imaging* system were back. Both of these companies had been in the spotlight of the *PittCon Editors' Awards* in years past. In addition, both Ardara Technologies, a manufacturer of quadrupole *m/z* analyzers in Pittsburgh, PA (http://www.ardaratech.com), and Bio-Rad Laboratories, manufacturer and support for the Ciphergen Biosystems, Inc.'s *ProteinChip®* Systems business and Surface Enhanced Laser Desorption/Ionization (SELDI) technology products (http://www.bio-rad.com), were present. The Informatics Division of Bio-Rad Laboratories produces the *KnowItAll* software (http://www.informatics.bio-rad.com). Syft™ Technologies Ltd. (Christchurch, New Zealand) (http://www.syft.com), producers of a selected ion flow tube mass spectrometer for volatile organic analyses such as those found in respiratory gases, were back at PittCon for the first time since 2005, which was their PittCon début.

The one notable absence from PittCon this year was Palisade Corp.—the publisher of *Mass Transit* (software used to convert between GC/MS and mass spectral library data file formats), *Benchtop PBM* (a program used to do library searches of GC/MS data against the Wiley Registry of mass spectral data), and *Palisade Complete* EI mass spectral database. Palisade has been at every PittCon since this report first appeared in the *Journal of the American Society for Mass Spectrometry* in 1995.

There were eight PittCon-sponsored short courses pertaining to mass spectrometry. There were 164 abstracts that contained "mass spec" in their titles. This ranged from "Mass Spectrograph with Faraday-Strip Array Detection for Ambient Mass Spectrometry" presented by Gregory D Schilling, Department of Chemistry, Indiana University, and coauthored with Charles J Barinaga, Pacific Northwest National Laboratory, James H Barnes, IV, Los Alamos National Laboratory, M Bonner Denton, University of Arizona, Gary M Hieftje, Indiana University, David W Koppenaal, Pacific Northwest National Laboratory, and Roger P Sperline, University of Arizona in the session entitled Mass Spectrometry: Applications in Homeland Security and Advances in New Instrumentation presided over by Susan V Olesik, Chemistry Department, Ohio State University, at the top of the list to A Quantitative Approach to Investigate Peptide Release from Neuronal Cells Using Microfluidics Combined with Mass Spectrometry presented by Ming Zhong, University of Illinois, Urbana-Champaign, with coauthors Kyubong Jo and Jonathan V Sweedler, both also from the University of Illinois, Urbana-Champaign, in the session entitled Analysis in Capillaries and Microchips at the bottom of the list.

It was also interesting to note that for the second straight year the American Chemical Society's Analytical Chemistry Division held its spring program at PittCon rather than in conjunction with the Spring ACS Meeting, which was also held in New Orleans April 6–10. It was announced that on March 3 the Analytical Division's executive committee voted to continue to hold its spring program in conjunction with PittCon rather than the Spring ACS Meeting for the next three years.

The following is a company-by-company description of new instrumentation. As is always the case, there may be some companies that belong in this category that were overlooked, especially this year because of the limited time I was able to spend at the conference; however, with an exhibition the size of the Pittsburgh Conference on Analytical Chemistry, it is easy to overlook those that do not make a specific effort to be known, or those that may be on the periphery of the field. With 1,110 companies exhibiting, it is hard to get to every mass spectrometry product, all the press conferences and receptions, and all the mass spectrometry technical sessions.

ACD/Labs (Toronto, Ontario, Canada)

ACD/Labs (Advanced Chemistry Development), a developer of software used to store, retrieve, and manipulate spectral and chemical data for all types, has produced a number of different programs to aid in the interpretation of chromatography and mass spectral data. This year, they introduced ACD/*AutoChrom* for use with the Agilent LC–LC/MS ChemStation and the Waters *Empower 2* chromatographic data system. ACD/

AutoChrom interfaces to the instrument control portions of the two data systems to provide computer-assisted rational method development reducing method development-time to days rather than weeks. ACD/*AutoChrom* is unlike previous method development software systems in that it adapts to the work flow of the chromatographer. It can perform method optimization experiments, test column combinations, and vary buffer and solvent systems. ACD/*AutoChrom* uses the ACD/*IntelliXtract* peak matching algorithm for automated peak matching. This unique spectral-based peak matching algorithm makes peak tracking between screening experiments easy and a reality.

More information on all of the ACD/Labs product line can be found at http://www.acdlabs.com.

Agilent Technologies, Inc. (Santa Clara, CA)

GC and GC/MS were a high point for new product introductions by Agilent at PittCon 2008. Last year, Agilent introduced capillary flow technology on the *7890A* GC. This manifested itself in a number of ways; one of the most important was the ability to change GC columns in a GC/MS system without having to break vacuum on the mass spectrometer. This same technology is now being used for a GC × GC (2D GC or Comprehensive GC) system that does not require cryogenic focusing of the eluate from the first GC column going to the second column. Chromatographic peak widths produced by the second column are reported to be 600–1000 ms at half height of full maximum.

With the increased productive pressures in all types of GC/MS laboratories, there has been an increased demand for shorter analysis times. This usually means shorter chromatographic times. Shorter chromatographic times mean faster mass spectral data acquisition rates. These faster spectral acquisition rates mean less time in counting the ions that represent any single *m/z* value. To compensate for these weak signals, instrument manufacturers have been working to reduce the electrical noise in their systems. One of the primary sources of electrical noise in a mass spectrometer is in the device that detects the ions once they are separated according to their individual *m/z* values. This noise reduction is exactly what the Agilent *5975C Triple-Axis Detector* (TAD) does. This allows for the new detection limit specification of 400:1 for 1 pg of octafluoronaphthalene (OFN) injected onto the GC column. The TAD also introduces a triple-channel multiplier, which provides more amplification and longer life than previous multipliers. Agilent's new *Gain Normalized* optimization of the electron multiplier provides an optimal balance between ion count, linearity, and life expectancy. Gain Normalization also provides consistent detection limits as the electron multiplier ages and provides consistent ion counts between multiple GC/MS systems to allow for better understanding of correct operating conditions.

Agilent also introduced a new version of their Deconvolution Reporting Software (*DRS Ver. A.04.00*). Agilent DRS is an application for target compound analysis that combines results from Agilent ChemStation for GC/MS, the National Institute of Standards and Technology (NIST) *Automated Mass spectral Deconvolution and Identification System* (AMDIS), the 2005 version of the National Institute of Standards and Technology Mass Spectral Database (*NIST05*), and the *NIST Mass Spectral Search Program* into one easy-to-read automated report.

This new version of Agilent DRS provides quantitation of AMDIS deconvoluted results in the Agilent *MSD ChemStation's QEdit*. It also generates summary reports of both MSD ChemStation and AMDIS deconvoluted results. Users save time and produce more reliable results with Agilent's DRS. Complex data can be analyzed in as little as one minute of processing time per sample. Agilent DRS is more thorough than standard quantification and library search methods provided by ChemStation alone, and it finds additional targets not found by the conventional data system. Screening and quantitation can be performed in a single run, and there's no need to learn a separate software application.

At PittCon 2008, Agilent announced the sale of their 500th *6410* triple quadrupole mass spectrometer to professors Hugo Neels, Ph.D., and Adrian Covaci, Ph.D., Department of Toxicology, University of Antwerp, Belgium. Agilent also announced a B version of the *6410* that provides polarity switch (positive/negative ion detection) every 500 msec. The instrument also is reported to double the number of selected reaction monitoring (SRM) transactions that can be monitored in a single time period. The instrument now boasts a value of more than 10,000 SRM transactions per method.

Other enhancements to the Agilent tandem-in-space triple quadrupole and quadrupole–TOF mass spectrometers have to do primarily with ion cooling, which improved detection limits.

Applied Biosystems, Inc./MDS Sciex (Foster City, CA/Toronto, Canada)

Applied Biosystems/MDS Sciex introduced a Phase I and II metabolite identification platform based on their *4000 QTRAP*, which uses Ver. 2.0 of the *LightSight* software. This metabolite identification system speeds up metabolite detection by employing an SRM-triggered *Information Dependent Acquisition* (IDA) algorithm proprietary to ABI/Sciex. The company also exhibited its other popular mass spectrometers including their MALDI TOF–TOF tandem instrument.

Additional information about the *LightSight* software for metabolite identification from Applied Biosystems, Inc./MDS Sciex can be found at: https://products.appliedbiosystems.com/ab/en/US/adirect/ab?cmd=catNavigate2&catID=602162&tab=DetailInfo.

Bruker Daltonics Inc. (Billerica, MA; Bremen, Germany)

At PittCon 2008, Bruker Daltonics made five major product announcements.

- The *FlashFormula™ NALDI-TOF Solution* using nanotechnology-enabled targets for high-throughput molecular formula determination of small molecules employing matrix-free laser desorption ionization (LDI). Many of the small molecules that can be identified with NALDI-TOF are not easily analyzed using traditional MALDI and required LC/MS. Identification is facilitated using Bruker's *SmartFormula™* method that combines accurate mass measurement with a *True Isotope Pattern* (TIP) fitting algorithm for obtaining elemental compositions. *FlashFormula* is a name that reflects the speed and simplicity of elemental composition finding with a NALDI-TOF system. The dedicated 96-position NALDI targets have a form-factor compatible with all of Bruker's FLEX-series MALDI-TOF instruments. Small molecules are captured from liquid droplets onto the targets, an optional washing step removes salts and protein contaminants, and measurement takes a few seconds per sample, followed by automated data interpretation. Detection limits are compound dependent, but many molecules are reported to give impressive results at a low picogram level on target. A linear quantitation range of more than 3 orders-of-magnitude is claimed to be possible with the addition of known levels of an internal standard. The NALDI targets are developed and manufactured by Nanosys Inc. and are exclusively distributed by Bruker Daltonics under a collaboration agreement. Nanosys Inc., a privately held Palo Alto, California, company, is a leader in the development of nanotechnology enabled products utilizing high performance inorganic nanostructures. Nanosys has built one of the broadest technology platforms in the industry with approximately 500 patents and patent applications covering fundamental areas of nanotechnology. Additional information on Nanosys can be found at www.nanosysinc.com.
- The *micrOTOF™-QII*, a new generation transmission quadrupole–TOF tandem-in-space mass spectrometer (QqTOF) providing a resolving power (R) of up to 20,000 at a spectral acquisition rate 20 spectra sec^{-1} from fast LC and still provides a mass accuracy of 1–2 ppm. This new instrument can also take advantage of the *SmartFormula* software, described above, to combine accurate mass and isotopic patterns of both mass spectral and MS/MS data to determine the elemental composition of small molecules up to 1 kDa. The *micrOTOF-QII* has a high resolution extracted ion chromatogram (hrEIC) that provides 0.002 Da data for multiple target screening applications in environmental, food, and forensic analyses, where triple quadrupole instruments are typically used that provide no better than 0.1 Da results.
- The *MALDI-TDS™* (Top-Down Sequencing), a novel MALDI TOF/TOF system based on the *ultraflex III* TOF/TOF mass spectrometer for top-down sequencing, PEGylation site, and N/C-terminal assignments in protein drugs.
- A MALDI tissue scanning and imaging system employing the *apex®-ultra* FTMS, with a 7-Tesla magnet and a resolving power (R) of >900,000. Bruker's *SmartBeam* laser technology allows for 200 Hz laser repetition rates with spot sizes of <40 μm. The performance in the *m/z* region of 150–2,000 does not suffer from complications of matrix background cluttered spectra without the need for their prior tandem MS isolation.
- The next generation electron transfer dissociation (ETD) for *HCT-Ultra™* high capacity 3D quadrupole ion trap. ETD allows for top-down capabilities in proteomics. Bruker is claiming that the implementation of ETD on their high capacity 3D QIT provides 10–100 times the sensitivity obtainable with ETD in a linear quadrupole ion trap. Bruker claims that with a resolving power in their 3D QIT that will allow for the separation of 3+ and 4+ charge states and an upper *m/z* limit of 3,000 that their combination of proton transfer reaction (PTR) and ETD on the *HCT-Ultra* can be used for proteins with a mass of up to and greater than 12 kDa.

More information on all of the Bruker Daltonics line of mass spectrometers and software can be found at http://www.bdal.com. Although this is the same Web address used in last year's report, this is a different Web site from that reported in previous years.

John Wiley & Sons (Hoboken, NJ; Chichester, UK)

John Wiley continues to expand its position in mass spectrometry with both books and electronic databases of electron ionization mass spectra. Wiley had at least 20 different book titles on mass spectrometry at PittCon this year including *Introduction to Mass Spectrometry: Instrumentation, Applications and Strategies for Data Interpretation*, 4th ed., by J. Throck Watson and O. David Sparkman; Wiley: Chichester, UK, 2007, ISBN: 9780470516348; *Mass Spectrometry: Principles and Applications*, 3rd ed., by Edward de Hoffmann and Vincent Stroobant; Wiley: Chichester, UK, 2007, ISBN: 9780470033104 (not translated from French language as were the first two editions); 2nd ed.; Wiley: New York, 2001, ISBN:0471485659 (original French language edition, *Spectrométrie de masse*, © Dunod, Paris, 1999); 1st ed., de Hoffmann, E; Charette, J; Stroobant, V *Mass Spectrometry: Principles and Applications*; © Masson éditeur Paris, 1996; Wiley: New York, 1996, ISBN: 0471966967 (reviewed *JASMS* 8:1193) (original French language edition, *Spectrométrie de masse*, © Masson éditeur, Paris, 1994). *Fundamentals of Contemporary Mass Spectrometry* by Chhabil Dass (Wiley Interscience Series on Mass Spectrometry); Desiderio, DM; Nibbering, NM,

Series Editors; Wiley: New York, 2007, ISBN: 9780471682295 (reviewed *JASMS* 18(11):R1-R2).

Wiley is now the primary distributor of the Wiley Registry of Mass Spectral Data. This database and all of Wiley's other mass spectral databases are offered in proprietary formats for various instrument manufacturers' mass spectrometry data systems as well as the NIST format. Electronic searchable structures are now provided for the Wiley Registry and all other Wiley databases in the NIST and Agilent Technologies format. The following is a list of available Wiley EI mass spectral databases:

- *Wiley Registry of Mass Spectral Data*, 8th edition, ISBN:0-470-04785-2 (Wiley 8) and 8th edition with NIST05 ISBN:0-470-04786-0 (Wiley 8N) contain 399,389 and 522,384 electron ionization mass spectra, respectively.
- *Mass Spectra of Designer Drugs 2007*, Dr. Peter Roesner, Regional Department of Criminal Investigation Kiel, Kiel, Germany, ISBN:978-3-527-31979-4, contains 7,006 spectra of 6,029 compounds and 2,159 Kovats indices. A two-volume text set is also available for this database (ISBN:978-3-527-31538-3). *Mass Spectra of Designer Drugs 2008* was announced a few weeks after PittCon and contains 9,658 spectra of 8,300 compounds. This database will be offered on an upgradable basis.
- *Mass Spectra of Volatile Compounds in Food*, 2nd edition, Central Institute of Nutrition and Food Research (TNO), AJ Zeist, The Netherlands, ISBN:0-471-44056-6. *Mass Spectra of Organic Compounds*, Dr. Alexander Yarkov, Chemical Block, Moscow, Russia, ISBN:0-471-66773-0, contains 37,055 mass spectra.
- *Mass Spectral Collection: Geochemicals, Petrochemicals and Biomarkers*, 2nd edition, J. W. de Leeuw, Netherlands Institute of Sea Research, Texel, The Netherlands, ISBN:0-471-64798-5, contains 1,100 mass spectra.
- *Mass Spectra of Pharmaceuticals and Agrochemicals 2006*, Rolf Kühnle, ISBN:978-3-527-31615-1, contains 4,563 mass spectra.
- *Mass Spectra of Androstanes, Oestrogens and Other Steroids*, Professor HLJ Makin, St. Bartholomew's and the Royal London School of Medicine and Dentistry, London, UK, ISBN:0-471-44034-5, contains 2,500 electron impact mass spectra.

It should also be noted that there is a new edition of the *Mass Spectral Library of Drugs, Poisons, Pesticides, Pollutants and their Metabolites*, 2007 edition, along with a two-volume text set, *Mass Spectral and GC Data of Drugs, Poisons, Pesticides, Pollutants and their Metabolites* (Third, Revised and Enlarged Edition) by Hans H. Maurer, Karl Pfleger, and Arnin A. Weber (ISBN:978-3-527-32146-9). The hardcopy books are available without the electronic data (ISBN:978-3-527-31538-3). Previous editions of these data were known as the Pfleger/Maurer/Weber (PMW) database; however, this latest edition changes the order of the authors. Unlike the previous edition of the electronic format that were available only from mass spectrometer manufacturers as condensed spectra, this current version is provided with full spectra and like all the other electronic versions of Wiley mass spectral databases is in a variety of instrument company formats as well as the NIST MS Search Program's format. As with other Wiley databases, the new MPW database is provided with structures in an electric form for use with the NIST MS Search Program and the Agilent MSD ChemStation.

LECO Corp. (St Joseph, MI)

LECO made its first appearance at PittCon as a mass spectrometer company in 1996 with the introduction of *Pegasus* GC/TOFMS using the rapid detection TOF technology developed by the Michigan State University Mass Spectrometry Facility. In the ensuing twelve years, LECO has continued to grow as a TOF mass spectrometer company in both LC/MS and GC/MS. This growth has been as a result of acquisition and in-house product development. LECO became a pioneer in GC $\times$ GC and its use with mass spectrometry. Because of the rapid spectral acquisition rates of their original instrument and it successors, their TOF was an ideal marriage with GC $\times$ GC. The one thing that LECO lacked in the area of GC/MS was chemical ionization (CI). The *Pegasus* introduced in 1996 and all of its successors were electron ionization (EI) only instruments. At the ASMS Meeting in Indianapolis last year, LECO introduced the *TruTOF HT TOFMS*, a benchtop GC/MS offering both EI and CI with a data acquisition rate of 80 spectra sec^{-1}. This year was the first-time showing of the *TruTOF HT TOFMS* at PittCon. The instrument has an EI detection limit (sensitivity) specification for a full range acquisition of >10:1 for a mass chromatographic peak of *m/z* 284 ($[M + 2]^{+2}$) for 2 pg hexachlorobenzene (HCB) injected onto the column. The specification for CI is >10:1 for 10 pg of benzophenone using a mass chromatographic peak at *m/z* 183 (MH^+). No resolving power or resolution specification is provided but is assumed to be unit resolution throughout the *m/z* scale. This instrument uses the LECO *ChromaTOF*® software, which takes advantage of the high data acquisition rate to provide chromatographic peak deconvolution. The instrument was selected Strategic Directions International, Inc's. (SDi) *Instrument Business Outlook* as the "best new product from the 2007 ASMS meeting in Indianapolis.

ThermoFisher Scientific (Waltham, MA; San Jose, CA)

The mass spectrometry products from ThermoFisher are now branded as Thermo Scientific mass spectrometers. At ASMS 2007, it was announced that electron transfer dissociation (ETD) on the *LTQ*, announced at

PittCon just a few months earlier, would be available on the *LTQ* orbitrap and that it would be available as an upgrade to existing *LTQ* orbitraps. At PittCon this year, that announcement became a reality, and ETD for the *LTQ* orbitrap is now shipping. At the same time, the company announced the availability of matrix-assisted laser desorption/ionization (MALDI) on both the *LTQ Orbitrap XL* (resolving power (R) of 100K) and the *LTQ Discovery* (R of 30K) as well as the *LTQ FT Ultra* Fourier transform ion cyclotron resonance mass spectrometer (R of >750,000). This MALDI ion source used with the *LTQ XL* mass spectrometer and *ImageQuest* software for tissue imaging opens the possibility for the analysis of whole tissues and biological and polymer samples with minimum sample preparation. This MALDI source operates at reduced pressure and, due to a completely redesigned laser, exhibits better performance than previous models. By using the *LTQ* orbitrap with this new MALDI source, it is now possible to obtain MS^n on ions produced by MALDI.

ThermoFisher also introduced a new *IRQ* (3D QIT) GC/MS Series. As with the QIT products of the recent past, all of these instruments have external ionization providing EI, CI, and electron capture negative ionization (ECNI). The members of this series have the designation of *ITQ 700*™, *ITQ 900*™, and *ITQ 1100*™. The three models are differentiated by a number of factors, the main being the upper limit of the *m/z* range. This is 700 for the *ITQ 700*, 900 for the *ITQ 900*, and 1,100 for the *ITQ 1100*. The lower limit of the *m/z* range is 10 for all three instruments. The rate at which ions are scanned out of the trap is the same for all three instruments, 5,555 integer *m/z* units per second. All three instruments are offered as EI only with chemical ionization as an option. It appears that the CI option includes the PPNIC (pulsed-positive negative-ion chemical ionization) mode. MS/MS is standard only on the *ITQ 1100* but is available as a retrofittable upgrade for the *ITD 700* and *ITD 900*. The MS/MS option includes MS^n, Automated Collision Energy (ACE), and the patented Pulsed Q Dissociation Mode (PQD). Both the *ITD 700* and the *ITD 900* are provided with a 70-L sec^{-1} turbomolecular pump. Both are upgradable to a 250-L sec^{-1} pump, which is standard on the *IT 1100*. The vacuum probe interlock is also only standard on the *ITQ 1100* but is available as an upgrade on the other two models. The main differentiator for the *ITQ 700* is the GC. This model is provided with a *Focus GC*, which has no control other than through the data system and only a split/splitless injector. The *Focus GC* also has a much smaller footprint than the *Trace GC Ultra* provided with the other two models. The *Trace GC* allows for multiple injectors and additional GC detectors.

In addition, ThermoFisher Scientific showed at PittCon for the first time the *TSQ Quantum*, which was introduced at ASMS in Indianapolis last year. The *TSQ Quantum* is a GC triple quadrupole mass spectrometer with an *m/z* range of 10–3,000 and a scan rate of 5,000 integer *m/z* units per second. The system uses a single triple-flow turbomolecular pump. The instrument uses the *HyperQuad*™ *m/z* analyzer technology and the *Trace GC*.

More information about all of these and other products can be obtained at http://thermo.com, the Thermo Scientific Web site of ThermoFisher Scientific.

Waters Corporation (Milford, MA)

Last year at PittCon, Waters introduced a truly unique tandem-in-space mass spectrometer, the *Synapt High Definition MS*™ (*HDMS*™) system. This instrument positioned three of the earlier introduced T-wave devices in the traditional position of a collision cell that separated a transmission quadrupole (MS1) and a reflectron TOF mass spectrometer. These devices provide ion trapping ion mobility and the normal collision cell capability. The data shown with the *HDMS* was outstanding. This year, Waters introduced the *Synapt MS* system, which changes the concept of the tandem-in-space mass spectrometer almost as much as the *HDMS* did. The *Synapt MS* system has two of the T-wave devices in place but does not have the ion mobility cell. However, this platform is field upgradable to the *HDMS*. The *Synapt MS* system will replace the traditional high-end Q-TOF instrument that has been offered by Waters over the last several years. The ability for ion trapping and multiple stages of collisionally activated dissociation gives this instrument a lot of flexibility. If, at a later date, the need of the ion mobility stages becomes necessary, the laboratory only has to order the upgrade and have it installed.

And That's Not All . . .

This PittCon report on mass spectrometry is abbreviated compared to years past. That is partly due to the fact that I was only at the conference one day and partly because, as we all knew, the manufacturers could not continue at the pace that has dominated the last few years. I am looking forward to see what will be the new introductions at this year's ASMS meeting in Denver.